Folding channels for coarse-grained heteropolymer models

S. Schnabel, M. Bachmann, and W. Janke
Institut für Theoretische Physik, Universität Leipzig
Postfach 100920, D-04009 Leipzig, Germany

By means of multicanonical computer simulations [1], we investigate folding properties of proteinlike hydrophobic-polar heteropolymers employing a simplified model on mesoscopic scales [2,3]. In this physics-based approach, nonbonded pairs of monomers interact via specific monomer-type dependent Lennard-Jones potentials. Steric torsional barriers are taken into account by a chain's bending energy. The model is based on the hydrophobic effect and thus hydrophobic contacts are particularly favored allowing for the formation of a compact hydrophobic core. We analyze for three permuted hydrophobic-polar sequences the folding channels in the free-energy landscape and find typical folding characteristics known from real proteins: two-state folding, folding through intermediates, and functional metastability. For the identification of the folding channels, we compare equilibrium conformations with the respective folded conformations using a suitable order parameter, the angular overlap parameter [4].

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